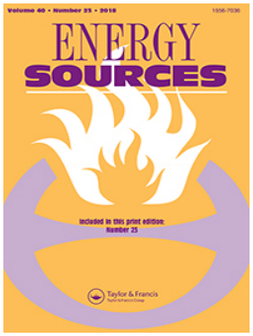

Energy Sources, Part A: Recovery, Utilization, and Environmental Effects

ISSN: 1556-7036 (Print) 1556-7230 (Online) Journal homepage: https://www.tandfonline.com/loi/ueso20

Emission spread from mass and energy exchange in the atmospheric surface layer: Two-dimensional simulation

Nurgali Zaurbekov, Allayarbek Aidosov, Nurbike Zaurbekova, Galym Aidosov, Gulzat Zaurbekova & Igilik Zaurbekov

To cite this article: Nurgali Zaurbekov, Allayarbek Aidosov, Nurbike Zaurbekova, Galym Aidosov, Gulzat Zaurbekova & Igilik Zaurbekov (2018) Emission spread from mass and energy exchange in the atmospheric surface layer: Two-dimensional simulation, Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 40:23, 2832-2841, DOI: 10.1080/15567036.2018.1511656

To link to this article: https://doi.org/10.1080/15567036.2018.1511656

Published online: 24 Aug 2018.

ENERGY SOURCES, PART A: RECOVERY, UTILIZATION, AND ENVIRONMENTAL EFFECTS
2018, VOL. 40, NO. 23, 2832–2841
https://doi.org/10.1080/15567036.2018.1511656

Taylor & Francis
Taylor & Francis Group

Emission spread from mass and energy exchange in the atmospheric surface layer: Two-dimensional simulation

Nurgali Zaurbekov[a], Allayarbek Aidosov[b], Nurbike Zaurbekova[c], Galym Aidosov[d], Gulzat Zaurbekova[e], and Igilik Zaurbekov[a]

[a]Almaty Technological University, Almaty, Kazakhstan; [b]Kazakh national University named after al-Farabi, Almaty, Kazakhstan; [c]Kazakh State Women's Teacher Training University, Almaty, Kazakhstan; [d]Kazakh national University named after al-Farabi, Research Institute of mathematics and mechanics, Almaty, Kazakhstan; [e]Kazakh national University named after al-Farabi, Department of computer science, Almaty, Kazakhstan

ABSTRACT

This article provides an original method for simulating the spread of hazardous emissions in the atmospheric surface layer in the event of emergencies The modeling process implies the development of a mathematical tool based on the partial differential equation (PDE) of turbulent diffusion. It is also based on a steady-state equation for determining the contaminant dispersion during an emergency with regard to the elapsed dispersion time, volumetric nature of the contamination source, wind speed. The model allows studying the changes in air composition that have occurred under various meteorological (wind speed and direction, temperature, fogs, precipitation, dust winds) and anthropogenous factors. An attempt was made to calculate the probable contamination area around the arbitrary system of sources with high contaminant concentration under unfavorable weather conditions. The original method for calculating the movement and dispersion of emissions allows forecasting the contaminant concentration level in the two-meter layer above the ground and the vertical concentration distribution with regard to the landscape, identified according to the meteorological data. Our model can be easily scaled on any territory; the entire line of complex landscape features was taken into account by introducing a model of weather statistics for the research region.

ARTICLE HISTORY
Received 11 June 2018
Accepted 25 July 2018

KEYWORDS
Atmosphere; dispersion of contaminants; ecology; emission; mathematical model; pollution

Introduction

Natural resources development, industrial construction, and city development entail air pollution (Fritz et al. 2015). Contaminants may be transferred over great distances and reach a specific region from far-away sources (Rosu, Constantin, and Georgescu 2016). Depending on its thermodynamic state, the atmosphere may either dilute the contaminants or accumulate them in lower layers, where the human activity is being performed (Aidosov et al. 2015). Therefore, meteorological aspects are of considerable practical importance when studying the behavior of contaminants in the atmospheric surface layer. The environmental impact of pollution may only be assessed reliably when the pattern of its spread is known.

Researchers studying the environmental effect of industrial disasters analyze the spread and effect of various chemical substances (gases, radionuclides, pesticides, heavy metals, etc.), as well as the various technologies applied to remove them from the atmosphere (Huimin et al. 2012; Lauenstein, Leung, and Hall-Spencer 2015). Models illustrating the spread of hazardous substances in the

CONTACT Nurgali Zaurbekov saul.yerbt@gmail.com Almaty Technological University, microdistrict Taugul-3, Abdramanov street, house 5, Almaty 8 707 739 05 63, Kazakhstan

Color versions of one or more of the figures in the article can be found online at www.tandfonline.com/ueso.

atmosphere are built to analyze the occurrence risk and probable aftermath of chemical disasters (Benchekroun and Chaudhuri 2014; Lee et al. 2014). There are researches (Late et al. 2016; Leuken et al. 2016) providing various classifications for the models of a spread of hazardous substance in the atmosphere. Problems related to the assessment of risks caused by industrial accidents are covered in (Aidosov et al. 2015; Kuzmanović et al. 2016; Zhao and Pei 2012).

Predicting gas dispersion and estimating source terms in atmosphere are required in many fields. There are few papers analyzing the stationary states, in particular – emission dispersion is determined by means of mathematical models that are based on fractional derivatives (Goulart et al. 2017). In cases, when one has to forecast the gas concentration distribution and/or assess the gas dispersion source, the following methods are applied: artificial neural network (ANN), particle swarm optimization (PSO), expectation maximization (EM (Sihang et al. 2018; Wang, Chen, and Zhao 2015)) machine learning algorithms (MLA), models, combined with thee Gaussian model (Denglong and Zhang 2016), computational fluid dynamics (Brzezinska et al. 2017).

In this paper, we have developed a method, based on the partial differential equation of turbulent diffusion, for determining the spread of contaminants in the atmospheric surface layer.

The offered stochastic model is intended for solving problems of environmental safety assessment in the following cases: when there are several pollution sources available; when there are environmental disasters, caused by natural phenomena or human activity; and when the elapsed dispersion time and wind speed are known. This method was tested around the Tengiz oil field. This method, unlike another model available in the literature, takes into account the entire line of complex landscape features by introducing a model of weather statistics for the research region. This allows putting it into application to study any scaled territory.

2. Modeling of the transfer and dispersion of hazardous emissions in the atmosphere

Our model was built with regard to the previously developed algorithms, the computational method (Aidosov et al. 2015) and the theory of partial differential equations (Goulart et al. 2017). The model takes into account the wind factor and unfavorable weather conditions.

The simulation process included the following stages:

1) modeling the transfer and dispersion of hazardous substances in the atmospheric surface layer and simulating the probable contamination pattern around the arbitrary contamination sources;

2) modeling the transfer and dispersion of hazardous substances in the atmospheric surface layer and simulating the probable contamination pattern around the environmental disasters caused by natural phenomena or human activity;

3) stochastic modeling of dispersion;

4) modeling the spread of active contaminants in the atmospheric surface layer;

5) analyzing the air condition with regard to the natural and anthropogenous factors.

The following analytical solution is intended for the algorithm building (Wilson and Sawford 1996):

$$q(x,y,z) = \frac{M}{4\pi x\sqrt{k_y k_x}} e^{-\frac{uy^2}{4k_y x}}\left[e^{-\frac{u(z+H)^2}{4k_z x}} + e^{-\frac{u(z-H)^2}{4k_z x}}\right] \tag{1}$$

The following steady-state equation (Kienle and Patterson 1997; Wilson and Sawford 1996) is determined for calculating the contamination pattern around one source:

$$\upsilon\frac{\partial q}{\partial x} + \vartheta\frac{\partial q}{\partial y} + w\frac{\partial q}{\partial z} = \frac{\partial}{\partial x}k_x\frac{\partial q}{\partial x} + \frac{\partial}{\partial y}k_y\frac{\partial q}{\partial y} + \frac{\partial}{\partial z}k_z\frac{\partial q}{\partial z} - \alpha q. \tag{2}$$

where: q – contaminant concentration; M – area source capacity; *υ, ν, w* – wind speed constituents along the axes (Cartesian plane); *x, y, z, kx, ky, kz* – exchange coefficient constituents; α – contaminant concentration coefficient.

Equation (2) was determined, according to the traditional forms of word shortening: wind direction is indicated on the *x*-axis

$$w = 0,\ \alpha = \ 0,\ k_x = 0,\ k_{ii} = k_i (i = x, y, z) \tag{3}$$

at the following boundary conditions (Diethelm 2010):

$$u_q = \ M\delta(y)\delta(z - H)\ at\ x = 0,\ q \to 0,\ at\ z = \infty,\ q \to 0,\ at\ |y| = \infty, k_z \frac{dq}{dz} = 0 \ \ at\ z = 0$$

Contamination process accelerates at the first phase of spread due to overheating. The real contamination source of the true height H was replaced with a higher fictitious source of height He in order to cover the acceleration effect:

$$\mathrm{H}e = H + \frac{1.5 w_0 R_0}{u}\left(2.5 + \frac{3.3 g R_0 \Delta \mathrm{T}}{\mathrm{T}_\alpha u^2}\right) \tag{4}$$

where: w_0 – initial velocity of gas discharge; R_0 –chimney mouth radius; $\Delta T = T - T_a$ – overheated gas temperature; T_a – absolute air temperature; g – gravitational acceleration.

Based on the differential calculus and computer algebra, a correction was made for ΔH limiting the plume rise at the zero wind speed (this corresponds with the physical significance of the problem) and not disrupting the monotony of the analytical solution (1) in regards to the speed module when H is replaced with He.

If we take the contaminant concentration are around an arbitrary system of sources as a superposition (1) of contamination areas around each source, we can calculate the critical wind speed module for a specified contamination level at each point of wind direction. In the light of the monotony of (1), dangerous concentrations may appear at any wind speed if its module does not exceed the established critical value.

If we accept the hypothesis regarding the normal distribution of the wind speed vector under the specified critical speed module, we can assess the probability of exceeding the set contamination level for the specified period at each distribution point under any wind condition by integrating a two-dimensional function of probability density. The angle may be integrated with any set accuracy. This approach allows calculating the contamination frequency fields in cases, when contaminant concentration is higher than any set value, as well as drawing the frequency contours. The solution involves only those sources that will contribute to the aggregate concentration at specified points.

Contaminant transfer and dispersion modeling was considered for two cases: short-term emission from a factory chimney and a thermal explosion of stored chemical substances. The model includes a partial differential equation (PDE) of turbulent diffusion, characterized by a partial derivative of concentration in time (Goulart et al. 2017):

$$\frac{\partial C}{\partial \tau} + v\frac{\partial C}{\partial x} = D_T\left(\frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) + \phi, \tag{5}$$

where: C – contaminant concentration in 1 m^3 of air; τ – time passed from the beginning of emission, v – wind speed; D_T – turbulent diffusion coefficient; φ – emission source function.

If we assume the contamination source to be semi-Gaussian, it will be described by the following equation:

$$\phi = \frac{j_0}{\rho}\exp\left(-\frac{\tau}{\tau_0} - \frac{x}{2R_0} - \frac{y^2}{R_0^2} - k_i\frac{z}{l_2}\right) \tag{6}$$

where: J_0 – bulk density of the first mass contaminant release, kg/(m· s), R_0 – chimney radius (or max cloud radius after the explosion), m; ρ – air density after contaminant release, kg/l, τ_0 – contaminant concentration coefficient (or cloud thickness coefficient), l_2 – chimney height (or the cloud height above the ground) (Figure 1).

Equation (1) is supplemented with initial and boundary conditions:

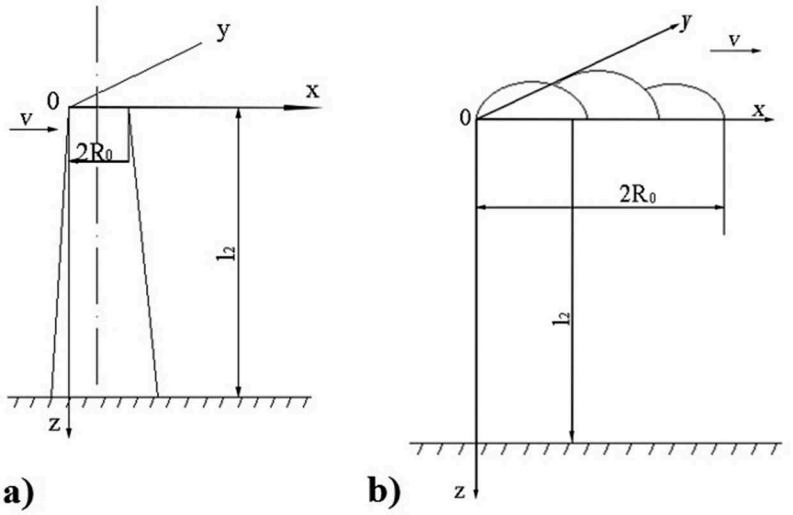

Figure 1. Basic dispersion model data: (a) emission from a chimney; (b) explosion.

$$C|_{t=0} = 0; C|_{x=0} = 0; \left.\frac{\partial C}{\partial y}\right|_{y=0} = \left.\frac{\partial C}{\partial y}\right|_{y=l} = 0; \left.\frac{\partial C}{\partial z}\right|_{z=l} = 0; C|_{z=l_2} = 0, \tag{7}$$

Where: l is the half-width of the wind layer.

At conditions (6) and (7), Equation (5) was solved by applying the Fourier integral transforms (to exclude the t variable) and the theory of complex variable functions.

For the sake of convenience, the final equation for estimating the concentration of the contaminant in the air is the following sum:

$$C = C_1 + C_2,$$

Where:

$$C_1 = A \sum_{k,m=1}^{n} \frac{B_k}{1+\alpha_{km}} \left\{ -\exp(-\overline{x-\tau}) + \exp\left(-\frac{D_T \lambda^2 k m^x}{v}\right) \times \right.$$
$$\left. \times \left[\begin{array}{c} \exp(-|\beta|) \text{ if } \beta < 0 \\ \exp(-|\beta|)\alpha_{km} \text{ if } \beta \geq 0 \end{array} \right] \cdot \cos\left(\frac{\mu_k}{l} y\right) \cos\left(\frac{\eta_m}{l_2} z\right),$$
$$C_2 = A \sum \infty k, m = n \frac{-B}{1+\alpha_{km}} \times$$
$$\times \left\{ -\exp(-\bar{x})[\exp(-\bar{\tau}) - \exp(\alpha_{km}\bar{\tau})] - \exp\left(-\frac{D_T \lambda^2 k m^x}{v}\right) \times \left[\begin{array}{c} \exp(\beta) - \exp(-\alpha_{\mathrm{km}}\beta)] \text{if } \beta < 0 \\ 0 \text{ if } \beta \geq 0 \end{array} \right] \right\} \times$$
$$\times \cos\left(\frac{\mu_k}{l_1} y\right) \cos\left(\frac{\eta_m}{l_2} z\right). \tag{8}$$

$$M = \int_0^{\infty} \int_V j_V dV d\tau. \tag{9}$$

The calculated data allows determining the max contamination time and place. This is especially important when it comes to damage control and recovery after accidents, including timely protection

of people and pets against the hazardous impact of contaminants and the environmental reconstruction.

Unlike the deterministic models applied to solve the contaminant dispersion problems and based on the causal relationship description, the offered model is based on the assumption that the future does not depend on the past. This assumption does not contradict the physical model; it implies that the considered object depends on the circumstances.

In our research, cloud model may be described as follows. At some air-filled point in space, there is forming a sphere-shaped moving mass of smoke, which contains a certain amount of contaminants. Starting at a certain (initial) moment in time, this cloud will move in a field of homogenous and steady turbulence. Contaminant distribution in the cloud that moves in a homogenous and isotropic atmosphere corresponds with the Gauss's law (Moody and Paik 1993):

$$c = \frac{G}{2 \cdot x \cdot \sigma^2(t)} \exp\left(-\frac{r^2}{2\sigma^2(t)}\right) \tag{10}$$

where: G –emission source capacity, $\sigma(t)$ – standard deviation of contaminant particles in the cloud, t – time passed from the beginning of the process;

$$r = \left(x^2 + z^2\right) \cdot 0,5; \tag{11}$$

where: x and z – coordinates (with an origin at the cloud center).

If we consider the contaminant cloud as a substance carrier, we should determine its geometrical configuration via the effective radius. In this case, the cloud is a horizontally equivalent circle with radius r. Its visible boundary should be characterized by an extreme concentration value C_i, which is equal for all points along the boundary r or $r(t)$.

According to the *Geometrical Probabilities*, there is another solution for a sphere with an r radius in a two-dimensional space:

$$a^2(t) = r^2(t)/4, \tag{12}$$

since boundary values for all visible points are accepted as equal, then

$$\left[2\pi \cdot \sigma^2(t)\right]^{-1} \exp\left[-\frac{r^2}{2\sigma^2(t)}\right] = const. \tag{13}$$

If we differentiate this expression in time, we will get the following:

$$d(r^2)/dt = (d(\sigma^2)/dt) \cdot \left[\left(r^2 - 2\sigma^2\right)/\sigma^2\right], \tag{14}$$

which becomes zero at $r^2 = 2\sigma^2$ (for a one-dimensional space).

The first part of the solution requires finding the probability P for a random point K falling into the plane domain S:

$$P = \iint_S \phi(\xi) dd. \tag{15}$$

The second part of the solution is related to the grid coverage problem, when the area consists of all points with integer coordinates. The probability of any point being covered at least by one circle within the largest unit square (grid element) is as follows:

$$l - \left(\frac{1 + 4 \cdot r}{1 + 4 \cdot r + \pi^2}\right). \tag{16}$$

If we calculate the volume of hazardous substances released into the atmosphere with regard to each substance, the following condition will repeat:

$$q_{sum.j} = q_{sc.j} + q_{b.j} = \frac{C_{sc.j} + C_{b.j}}{TLV_j} < 1 \tag{17}$$

where: $C_{sc.j}$ – deposition coefficient (substance j concentration after falling), $C_{b.j}$ –background concentration, TLV - threshold limit value.

Research object

The research model was selected to be the Tengiz oil field – an oil field located in northwestern Kazakhstan's low-lying wetlands along the northeast shores of the Caspian Sea. Research results were analyzed using the monitoring data published by the Kazgidromet Centre for Research and Development in 2016 (Republican state enterprise "Kazgidromet" under The Ministry of Energy of the Republic of Kazakhstan, 2016).

Results and discussion

The peculiarities of emission spread from several sources were studied with regard to weather conditions and wind direction. Different meteorological conditions were set with the following parameters: $\bar{u}$, v – average wind speed constituents by month along the axes (Cartesian plane); x', $0y'$, σu, and σv – are respective standard deviations; r – correlation coefficient; T –average air temperature (°C). The estimations were made in relation to sources with equal parameters: M = 1.4 kg/s, R_0 = 2 m, w_0 = 22 m/s, H = 100 m, ΔT = 100°C. However, the introduced method can be also applied in relation to the sources with different parameters. All simulations are based on the same average wind value. A point placed on each image stands for pollution sources. The 0.1 probability corresponds to 72 h.

In simulation *1*, there is only one active source with the following parameters: T = −16°C; ū = −0.57 m/s; v = −0.58 m/s; σv = 1.3 m/s; r = 0.14. The zero contour outlines the area (Figure 2a), where the probability of contamination level being higher than it is accepted is close to 0. Contour *1* outlines the area, where high contaminant concentration remains at least for 108 h per month. Simulation 2 is similar to the simulation 1 but is based on other parameters: σu = 1 m/s, σv = 6 m/s. Since the range of *v* values is wide, there are two areas with the highest level of pollution at the max elapsed dispersion duration – 391 h and 336 h (Figure 2b). Simulations with a single source show that areas with dangerous concentrations in certain meteorological situations may occur only in the direction of the dominant wind. *In simulation 3*, there are six active sources; the situation

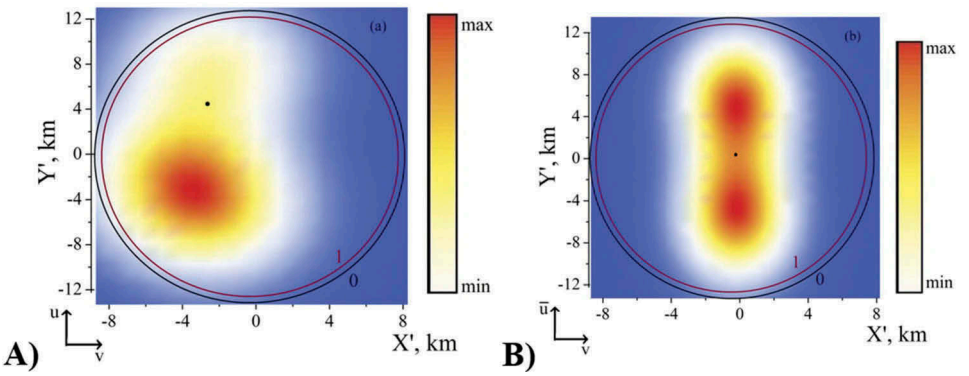

Figure 2. Probable area of contamination from a single active source at (a) T = −16°C; ū = −0.57 m/s; v = −0.58 m/s; σv = 1.3 m/s; r = 0.14; (b) T = −16°C; ū = −0.57 m/s; v = −0.58 m/s; σu = 1 m/s, σv = 6 m/s; r = 0.14. ū, v – average wind speed constituents by month along the axes (Cartesian plane).

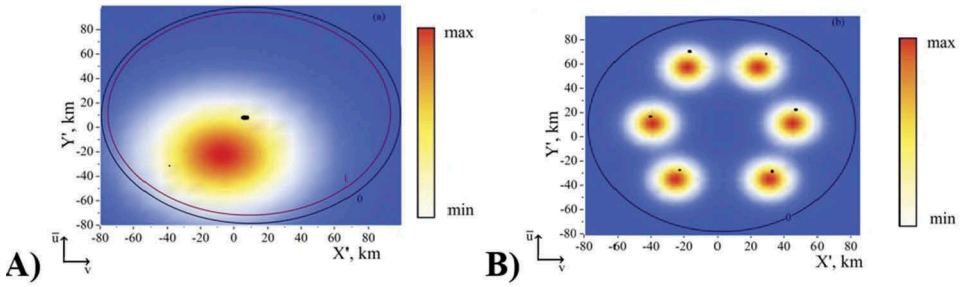

Figure 3. Probable area of contamination from (a) 6 sources, (b) 6 sources, two thereof are located at some distance (c) sources located irregularly. ū, v – average wind speed constituents by month along the axes (Cartesian plane).

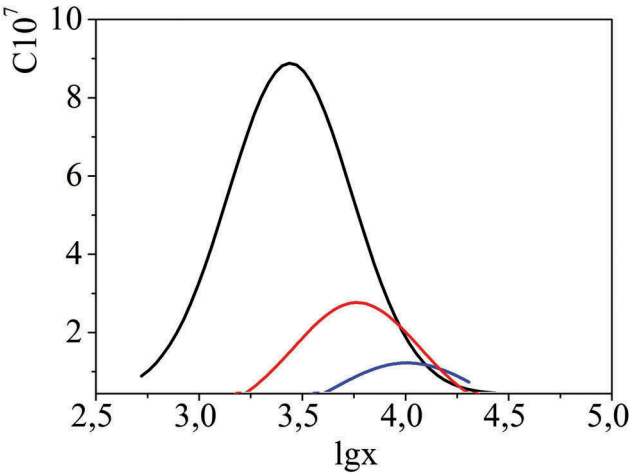

Figure 4. Dependency on wind speed.

is similar to the simulation 1. Sources are located near one another (Figure 3a). Thus, general pollution pattern is similar to that we calculated for the case with one source (Figure 2b). *In simulation 4, six* sources (Figure 3b) are placed at the apexes of a regular hexagon. They are located at such a distance from each other that contamination areas around them do not overlap. The superposition of dangerous areas covers a vast area (zero contour).

At the wind speed of 20 m/s, hazardous substances can spread at a distance four times greater than at v = 5 m/s. Thus, contamination level will be four times lower (from $5.15 \cdot 10^{-7}$ at v = 5 m/s to $1.44 \cdot 10^{-7}$ at v = 20 m/s). The ground level of contamination and the location of maxima largely depend on the chimney height (Figure 4). If we accept the chimney height to be two times higher (200 m instead of 100 m), max contaminant concentration at the ground level will be reduced by seven times. At the same time, the distance of emission spread from the chimney will be increased by four times. Similar results were obtained by the turbulent-diffusion equations solved to analyze the SO_2 concentration profile by time (Chen et al. 2017; Ebrahimzadeh and Shahsavand 2014).

The estimated model parameters are in Table 1. Basic data: elapsed dispersion time is 50, 100, and 150 s, respectively; cloud ($R \approx 120$ m) is entering the S area of 48.000 m^2; average wind speeds are: U_{av} = 1.0 m/s (α = 0.1) and U_{av} = 2.0 m/s (α = 0.25); the initial contaminant concentration – $C_{0.}$ For $U_{av} = 1.0m/cuu = 50s$; $\bar{U} = 0.1$; $(\overline{U'})^2 = 0.01$; According to (10); $\sigma^2(t) = 0.0150^2 = 25m^2$; $\sigma(t) = 5m$. Based on (8), the value of contaminant concentration at the cloud center *(r(t) = 0)* is found by the following formula:

Table 1. Data for the stochastic model of contaminant dispersion.

	U_{av} = 1.0 m/s, Ū = 0.1			U_{av} = 2.0 m/s, Ū = 0.5		
Estimated model parameters	t = 50s	T = 100s	t = 150s	t = 50s	t = 100s	t = 150s
1. Wind gustiness, α	0.1	0.1	0.1	0.25	0.25	0.25
2. L distance to the area contour, m	50	100	150	100	200	300
3. Contaminant dispersion	25	100	225	625	2500	5625
4. Squared error, σ(t)	5	10	15	25	50	75
5. Effective cloud radius, r(t)	10	20	30	50	100	150
6. Contaminant concentration at the cloud center, *C*	0.0064	0.0016	0.0007	0.00025	0.00006	0.00003
7. Concentration at the cloud border, *C*	0.00087	0.0002	0.000096	0.00064	0.000009	0.000004
8. Probability of a cloud entering this contour, (P)	1	1	1	0.7533	0.039	0.0047
9. Coverage percentage (P_2)	0.88	0.94	0.96	0.975	0.987	0.992
10. Probable concentration in the contour (P_1*P_2)	0.88	0.94	0.96	0.734	0.039	0.005

$$C_1 = \frac{C_0}{2 \cdot \pi \cdot 25} \exp\left(-\frac{0}{2 \cdot 25}\right) = 0.0064 \tag{18}$$

Let's consider the two-dimensional spread of a substance (aerosol) in the atmospheric lower layer, where the chain of its transformation from one chemical state to another consists of three links, according to the Michaelis-Menten theory (Bezerra, Pinto, and Fraga 2016). Let's assume that the free chemical substance and air first produce an air mixture (compound) in a reversible reaction, which in turn irreversibly disintegrates and again forms a free chemical substance and a product. Schematically, this reaction can be represented as follows:

$$S + E \overset{k_1}{\underset{k_{-1}}{\rightleftarrows}} SE \xrightarrow{k_2} P + E, \tag{19}$$

where: S, E, SE, P are the substrate (air), chemical substance, air mixture, and product, respectively; k_1, k_{-1} is the rate of the forward and backward reactions; k_2 is the rate of the mixture disintegration reaction.

Only the number of reagents that actually participate in the reaction are considered as the active reagents. If the concentration of the substrate, chemical substance, mixture, and a product are denoted by s, e, se, and p, respectively, then, according to the law of mass action,

$$\frac{ds}{dt} = -k_1 se + k_{-1} c, \frac{de}{dt} = -k_1 se + (k_1 + k_{-1})c, \frac{dc}{dt} = k_1 se - (k_1 + k_{-1})c, \frac{dp}{dt} = k_2 c \tag{20}$$

The Equation (20) system can be expressed with regard to diffusion, description whereof is based on the balance of the reagent φ:

$$\frac{\partial \phi}{\partial t} = -f + D\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right), \tag{21}$$

Where: D – diffusion coefficient.

Let us consider a two-dimensional layer of the air mixture with a unit thickness, wherein the chemical substance undergoes the process of diffusion. The air diffusion and reagent diffusion coefficients shall be denoted by D_r and D_f, respectively. The balance equations for the concentration of air, reagent, and air-reagent mixture are as follows:

$$\frac{dC}{dt} = f + D_r \Delta C, \quad \frac{dC_f}{dt} = -f + D_f \Delta C_f \tag{22}$$

$$\frac{dC_r}{dt} = f + D_r \Delta C_r \ \left(\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \tag{23}$$

where: C_r, C_f – reagent and air-reagent mix concentration. Equation (20) can be simplified with the following function ($k_2 = 0$):

$$f = k_1 C_f C - k_{-1} C_r \tag{24}$$

If we take into account the contaminant transfer by air in OX and OY directions with the u and v speeds, respectively, then

$$\begin{aligned} &\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + f = D_r \Delta C, \frac{\partial C_f}{\partial t} + u\frac{\partial C_f}{\partial x} + v\frac{\partial C_f}{\partial y} - f = D_f \Delta C_f, \\ &\frac{\partial C_r}{\partial t} + u\frac{\partial C_r}{\partial x} + v\frac{\partial C_r}{\partial y} + f = D_f \Delta C_r \end{aligned} \tag{25}$$

The Equation (25) describes the spread of the active substance with regard to diffusion, the chemical reaction and its transfer by air.

Unlike the model (Benchekroun and Chaudhuri 2014; Sarkkola et al. 2009; Shunxiang et al. 2015), our model takes into account several contamination sources and the landscape features. Thus, it allows forecasting the pollution level at the specified area if the elapsed dispersion time and wind speed are known.

Research results confirm the conclusion made by the Kazgidromet Centre for Research and Development – ground level concentrations of nitrogen dioxide, hydrogen sulfide and sulfur dioxide are rising insignificantly around the Tengiz Oil Field. Dispersion assessment has revealed that the highest contamination level can be recorded in the area with the released nitrogen dioxide.

Conclusion

This article provides a model of contaminant transfer and dispersion in the atmospheric surface layer, as well as a method for calculating the probable contamination area around the arbitrary system of contamination sources. The introduced model takes into account several contamination sources and the landscape features; thus, it allows forecasting the pollution level at the specified area if the elapsed dispersion time and meteorological (wind speed and direction, temperature, fogs, precipitation, dust winds) factors are known. The introduced method is intended for calculating the contaminant concentrations in a two-meter layer above the ground, as well as the vertical concentration distribution.

Funding

This research is supported by a Grant for Research and Development of the Ministry of Education and Science of the Republic of Kazakhstan, Budgetary program: 055 "Research and (or) Development", Subprogram: 101 "Grant Funding."

References

Aidosov, A. A., G. A. Aidosov, N. S. Zaurbekov, and G. I. Azhiyeva. 2015. *Model assessment of the technological load of environmental components in an oil and gas mining region*, 160. Volkova EV: Almaty.

Benchekroun, H., and A. R. Chaudhuri. 2014. Transboundary pollution and clean technologies. *Resource and Energy Economics* 36 (2):601–19. doi:10.1016/j.reseneeco.2013.09.004.

Bezerra, M. F., P. A. Pinto, and I. A. A. Fraga. 2016. Dias Enzyme inhibition studies by integrated Michaelis–Menten equation considering simultaneous presence of two inhibitors when one of them is a reaction product. *Journal Computer Methods and Programs in Biomedicine* 125 (C):2–7. doi:10.1016/j.cmpb.2015.12.013.

Brzezinska, D., and A. S. Markowski. 2017. Experimental investigation and CFD modelling ofthe internal car park environment in case of accidental LPG release. *Process Safety and Environmental Protection* 110:5–14.

Chen, M.-Y., Y.-P. Cheng, H.-X. Zhou, L. Wang, F.-C. Tian, and K. Jin. 2017. Effects of igneous intrusions on coal pore structure, methane desorption and diffusion within coal, and gas occurrence. *Environmental & Engineering Geoscience* XXIII (3):191–207. doi:10.2113/gseegeosci.23.3.191.

Denglong, M., and Z. Zhang. 2016. Contaminant dispersion prediction and source estimation with integrated Gaussian-Machine learning network model for point source emission in atmosphere. *Journal of Hazardous Materials* 311:237–45. doi:10.1016/j.jhazmat.2016.03.022.

Diethelm, K. 2010. *The analysis of fractional differential equations: An application-oriented exposition using differential operators of caputo type*. Berlin, Heidelberg: Springer-Verlag.

Ebrahimzadeh, E., and A. Shahsavand. 2014. Energy sources simulation of environmental pollution due to SO2 dispersion. *Energy Sources, Part A* 36:2095–105. doi:10.1080/15567036.2011.559525.

Fritz, B. J., J. M. Barnett, S. F. Snyder, L. E. Bisping, and J. P. Rishel. 2015. Development of criteria used to establish a background environmental monitoring station. *Journal of Environmental Radioactivity* 143:52–57. doi:10.1016/j.jenvrad.2015.02.010.

Goulart, A. G. O., M. J. Lazo, J. M. S. Suarez, and D. M. Moreira. 2017. Fractional derivative models for atmospheric dispersion of pollutants. *Physica A* 477:9–19. doi:10.1016/j.physa.2017.02.022.

Huimin, L., Z. Xuezhi, C. Haiping, H. Shunxiang, L. Feng, and W. Gang. 2012. Numerical simulation and field experiment validation of atmopheric pollution chemical accidents based on canopy model. *Procedia Environmental Sciences* 12 (A):30–37. doi:10.1016/j.proenv.2012.01.243.

Kienle, A., and M. S. Patterson. 1997. Improved solutions of the steady-state and the time-resolved diffusion equations for reflectance from a semi-infinite turbid medium. *Journal of the Optical Society of America* 14 (1):246–54.

Kuzmanović, M., J. López-Doval, N. Castro-Català, H. Guasch, M. Petrović, I. Muñoz, A. Ginebreda, and D. Barceló. 2016. Ecotoxicological risk assessment of chemical pollution in four Iberian river basins and its relationship with the aquatic macroinvertebrate community status. *Science of the Total Environment* 540:324–33. doi:10.1016/j.scitotenv.2015.06.112.

Late, M., R. Meroney, M. Yataghene, H. Fellouah, F. Saleh, and M. Boufadel. 2016. On the use of numerical modelling for near-field pollutant dispersion in urban environments – A review. *Environmental Pollution* 208 (A):271–83. doi:10.1016/j.envpol.2015.07.039.

Lauenstein, G., K. Leung, and J. Hall-Spencer. 2015. The global importance of regional studies in marine science: Trans-boundary pollutants matter. *Regional Studies in Marine Science* 2:A1–A2. doi:10.1016/j.rsma.2015.10.001.

Lee, J., J. Kim, K. Lee, M. Belorid, P. Beeley, and J. Yun. 2014. Assessment of wind characteristics and atmospheric dispersion modelling of 137Cs on the Barakah NPP area in the UAE. *Nuclear Engineering and Technology* 46 (4):557–68. doi:10.5516/NET.09.2014.029.

Leuken, J., A. Swart, A. Havelaar, A. Pul, W. Hoek, and D. Heederik. 2016. Atmospheric dispersion modelling of bioaerosols that are pathogenic to humans and livestock – A review to inform risk assessment studies. *Microbial Risk Analysis* 1:19–39. doi:10.1016/j.mran.2015.07.002.

Moody, M. V., and H. J. Paik. 1993. Gauss's law test of gravity at short range. *Physical Review Letters* 70:1195. doi:10.1103/PhysRevLett.70.4034.

Republican state enterprise "Kazgidromet" under The Ministry of Energy of the Republic of Kazakhstan. 2016. Letter of information on the state of environment. kazhydromet.kz/ru/bulleten/okrsreda?year=2016.

Rosu, A., D. E. Constantin, and L. Georgescu. 2016. Air pollution level in Europe caused by energy consumption and transportation. *Journal of Environmental Protection and Ecology* 17 (1):1–8.

Sarkkola, S., H. Koivusalo, A. Laurén, P. Kortelainen, T. Mattsson, M. Palviainen, S. Piirainen, M. Starr, and L. Finér. 2009. Trends in hydrometeorological conditions and stream water organic carbon in boreal forested catchments. *Science of the Total Environment* 408:92–101. doi:10.1016/j.scitotenv.2009.09.008.

Shunxiang, H., L. Feng, Z. Qingcun, H. Fei, Z. Jiang, and W. Zifa. 2015. Modeling and Optimal Control of Atmospheric Pollution Hazard in Nuclear and Chemical Disaster. *Procedia IUTAM* 17:79–90.

Sihang, Q., B. Chena, R. Wanga, Z. Zhua, Y. Wangc, and X. Qiua. 2018. Atmospheric dispersion prediction and source estimation of hazardous gas using artificial neural network, particle swarm optimization and expectation maximization. *Atmospheric Environment* 178:158–63. doi:10.1016/j.atmosenv.2018.01.056.

Wang, B., B. Chen, and J. Zhao. 2015. The real-time estimation of hazardous gas dispersion by theintegration of gas detectors, neural network and gas dispersionmodels. *Journal of Hazardous Materials* 300:433–42. doi:10.1016/j.jhazmat.2015.07.028.

Wilson, J. D., and B. L. Sawford. 1996. Review of Lagrangian stochastic models for trajectories in the turbulent atmosphere. *Boundary-Layer Meteorology* 78:191–210. doi:10.1007/BF00122492.

Zhao, Y., and Y. Pei. 2012. Risk evaluation of groundwater pollution by pesticides in China: A short review. *Procedia Environmental Sciences* 13:1739–47. doi:10.1016/j.proenv.2012.01.167.